SUSAN REMPE, Ph.D.

Principal Member of the Technical Staff
Sandia National Laboratories
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RESEARCH INTERESTS

Biomolecular structure-function relationships, ion channel permeation, membrane biophysics, enzyme binding, solvation & transport theory, water interfacial structure, clathrates, ab initio molecular simulations.

PROFESSIONAL PREPARATION

B.A. History & German (Premedical Concentration), Columbia University, NY 1987
B.A. Chemistry, U of Montana, MT 1989, *Research Advisor*: Dr. Richard J. Field
M.S. Chemistry, U of Washington, WA 1993
Ph.D. Chemistry, U of Washington, WA 1998
Thesis Topic: Potential energy surfaces for vibrating hexatomic molecules.
Thesis Advisor: Dr. Robert O. Watts

POSITIONS

Principal Member of the Technical Staff, Sandia National Laboratories, 2006-present
Senior Member of the Technical Staff, Sandia National Laboratories, 2001-2006
Postdoctoral Fellow, Theoretical Division, Los Alamos National Laboratory, 1999-2001
Visiting Research Scholar, U of Melbourne, Australia, 1996
Graduate Research Associate and Teaching Assistant, U of Washington, 1990-1998
Undergraduate Teaching Assistant, U of Montana, 1988-1990

HONORS & AWARDS

R&D 100 Award for research and development of "Biomimetic Membranes for Water Purification" (2011)
Employee Recognition Award for Individual Technical Excellence, Sandia (2011)
Award for Excellence, Laboratory Directed Research & Development, Sandia (2010)
Article chosen as dedicated feature on *Chem. Phys. Lett.* journal web site (2010)
Spot Awards for Exceptional Service, Exemplary Technical Work, Project Leadership ('08, '09, '10, '11)
Invited Speaker representing Science & Technology, Fall Leadership Forum for Sandia Executives (2007)
Research highlighted by the Biophysical Society as a *New & Notable* article (*Biophys. J.* (2007) 93:1091-92)
Sandia President's Volunteer Service Award for Coaching Kirtland Aquatic Club (2007)
Fellow of the American Academy of Nanomedicine (2006)
Young Investigator Award, American Academy of Nanomedicine (2006)
Research showcased in Sandia Research Program Review, Executive Report to Congress (2006)
Featured in *SNL Lab News, NanoWorld News, Alb. Tribune, SNL Research Quarterly, New Scientist* (2006)
Profiled in *New Mexico Woman Magazin*e as Outstanding Sandia Scientist (2004)
Women's Wall of Fame, Sandia National Labs (2004)
Research highlighted in *Chemical and Engineering News* 78:42 (2000)
DOE Educational Science Prize, U of Washington (1995)
Association for Women in Science Graduate Scholarship, U of Washington (1992)
Shell Graduate Research Fellowship, U of Washington (1992)
Ringold Outstanding Graduate Student Fellowship, U of Washington (1990-1996)
American Institute of Chemists Undergraduate Dept. Award, U of Montana (1990)
American Chemical Society Undergraduate Departmental Award, U of Montana (1990)
National Science Foundation Summer Undergraduate Research Grant, U of Montana (1989)
Baccalaureate Speaker, Columbia U (1987)
Pindyck Outstanding Undergraduate Academic Scholarship, Columbia U (1983-1987)

SYNERGISTIC ACTIVITIES

Organizer:

- Organizer & Chair, Telluride Science Research Center Workshop on "Ions in Aqueous Solutions and Molecular Biology: Theory, Simulation, Modeling" with T. Beck and L. Pratt, 2010 & 2012
- Organizer and Chair, Sandia's Annual Bioscience & Technology Conference with V. Vandernoot, 2009
- Organizer and Host, Sandia's Bioscience Symposium, 2007-current
- Organizer and Chair, International Symposium on "Ions in Complex Environments" with B. Roux, American Chemical Society Meeting in Washington, DC, 2005
- Chair, Symposium on "Classical and Statistical Studies of Solvation," Pacifichem Conference, Hawaii, 2005

Reviewer:

- Regularly review articles for *PNAS, J Gen Physiol, JACS, Biophysical J*, *J of Chemical Physics*, *Biophysical Chemistry*, *J of Physical Chemistry, J of Amino Acids, Phys Rev Lett, Phys Chem Chem Phys., BBA - Biomembranes*
- Regularly review proposals to *Petroleum Research Fund (ACS), DoE SBIR*
- Reviewer, Netherlands Foundation for Fundamental Research on Matter, 2011
- Member, first NSF Study Section on Chemistry of Life Processes, 2009
- *Ad hoc* reviewer, NSF (2010-current)
- *Ad hoc* reviewer, NIH Challenge Grants in Health and Science Research, 2009

Technical Advances:

- Technical Advance SD-1175 "Biomimetic membranes for water desalination" (2010)
- Provisional patent app. (Ser. No. 61/390,041) "Biomimetic membranes for water desalination" (2010)

Teaching:

- Developer and Teaching Assistant, UW's First Computational Chemistry Course with Profs. Hannes Jonsson, Rick Heller, Bill Reinhardt, 1993-1996 (won DOE Prize for Science Education)
- Computational exercise on molecular vibrations published in *The Chemical Educator* (1998)
- Teaching Assistant for General, Organic, and Physical Chemistry labs and lectures

Professional Memberships:

- Biophysical Society, American Chemical Society, Electrochemical Society, American Industrial and Chemical Engineers Society, American Academy of Nanomedicine, American Physical Society

Citizenship:

- Steering Committee Member, NIH Nanomedicine Center, 2006 –2009
- Member, SNL Bioscience Center committees: Diversity, Postdocs, NanoBio Strategy, 2007
- Member, Sandia Internal (LDRD) Proposal Reform Committee, 2004
- Member, Research Library Advisory Board, Los Alamos National Laboratory, 1999-2001

Journal Editor:

- Guest Editor, Special issue on "Ions" with B. Roux for *Biophysical Chemistr*y, 2006

Extracurriculars:

- Amateur Concert Pianist, performed at UNM Keller Hall 2003 (Spring & Fall), 2006, 2009
- Volunteer Swim Coach and Official (2004 – current)
- Whitewater kayaker and backcountry skier

POSTDOC & STUDENT COLLABORATORS: Dian Jiao, David Rogers, Ryan Davis, Adrian Schiess, Marielle Soniat (visiting grad student from UNO), Sameer Varma (U S Florida), Dubravko Sabo (NYU), Jacalyn Clawson (GlaxoSmithKline), Chris Lorenz (King's College), Jessica Lambert (Bernalillo high school)

SELECTED INVITED RESEARCH TALKS:
Over 65 invited research presentations.

2012 Workshop on ions & molec biology, Telluride
2012 Gordon Research Conf. on water, NH
2011 MRS Nanomaterials symposium, Boston
2011 U of S Florida physics colloquium, Tampa
2011 UNM Health Sciences Center, Albuquerque
2011 Ion channel biophysics workshop, Telluride
2011 Materials science external review, SNL
2010 Pacifichem Liquid interfaces symposium, HI
2010 Workshop on ions & molecular biology, Telluride
2010 DTRA division chief site-visit, Albuquerque
2010 EFRC workshop, Santa Fe
2010 American Water Works Assoc., Albuquerque
2010 NIH Nanomedicine Centers review, CA
2009 Hope College, WI
2009 Calvin College, WI
2009 Ion channel biophysics workshop, Telluride
2009 ACS Polarizable force fields symposium, SLC
2009 BPS Permeation & transport subgroup, Boston
2009 Weill (Cornell) Medical College, New York City
2009 Bioscience and Technology forum, Albuquerque
2008 MERCURY, Keynote speaker, Hamilton College
2008 U Maryland-College Park
2008 International School for Advanced Studies, Italy
2008 Wolfgang Pauli Institute, Vienna
2008 U Minnesota, Minneapolis
2008 AAAS Southwest regional meeting, Alb.
2007 Brandeis U., MA
2007 Nano-bio workshop on membranes, UI-UC
2007 Dupont briefing, Albuquerque
2007 NIH Nanomedicine Center review, Indianapolis
2007 NIH 8 Nanomedicine Centers review, Bethesda
2007 BPS workshop on ion channels, Baltimore
2007 Rush U. Medical Center, Chicago
2007 UNM Health Sciences Center, Albuquerque
2007 Bioscience Center external review, Albuquerque
2006 Materials Research Society (MRS), Boston
2006 UI-Urbana-Champaign
2006 NIH Nanomedicine Center review, UI-UC
2006 Americ. Acad. of Nanomedicine, Wash., DC
2006 The Mind Institute, UNM, Albuquerque
2006 Sandia-Livermore seminar, Livermore
2005 Pacifichem Interfaces symposium, HI
2005 Pacifichem Solvation symposium, HI
2005 AIChE, Cincinnati
2005 Pacific Northwest National Laboratory
2004 Beckman Institute, UI-UC
2004 Electrochemical Society, HI
2003 U of Houston
2003 Electrochemical Society, Paris
2001 Carleton College, MN
2001 U Montana, Missoula, MT
2001 Cal State, Long Beach
2001 ICCN Computational nanoscience, NC
2001 Sandia National Labs, Surface science, Alb.
2001 ACS Molecular aq. environments, San Diego
2000 Motorola, Los Alamos
2000 Pacifichem Ion channels symposium, HI
2000 NIST Thermophysical properties, Boulder
2000 ACS Frontiers in biophysical theory, Wash., DC
1998 Los Alamos National Laboratory
1998 Sandia National Labs, Computation Center, Alb.
1995 DOE Awards ceremony, Washington, D

RECENT FUNDED RESEARCH ACTIVITIES:

- DTRA JSTO-CBD (#CBS.FATE.03.10.SN.002), "Developing a molecular understanding of water-CWA-surface interactions," **co-PI**, $0.6M/1.5yrs (2/2010-9/2011).
- Sandia LDRD/New Directions, "K^+ channels: On/off switches of innate immune responses," **PI**, $1.3M/3 yrs (10/01/2008-9/30/2011).
- Sandia LDRD/Strategic Partnerships, "Multivalent interactions with charged lipids," **PI**, $50K/6mos (3/30/2011-9/30/2011).
- Sandia LDRD/Enabling Predictive Simulations, "Effects of morphology on ion transport in ionomers for energy storage," **co-PI**, $3M/3yrs (10/01/2009-9/30/2012).
- Sandia LDRD/Environment, Climate, Infrastructure, "Programmable nano-materials for reversible CO_2 sequestration," **co-PI**, $1.8M/3yrs (10/01/2009-9/30/2012).
- Sandia LDRD/Strategic Partnerships, "Biotechnology development for biomedical applications," **sub-project PI**, $400K/6mos (3/15/2010-9/15/2010).
- Sandia LDRD/Environment, Climate, Infrastructure, "Understanding and optimizing water flux and salt rejection in nanoporous membranes," **PI**, $1.5M/3yrs (10/01/2007-9/30/2010).
- NIH Nanomedicine Roadmap, "Design of biomimetic nanoconductors," **Sandia sub-project PI**, $6.3M/5yrs (10/01/2005-9/30/2010).

SELECTED PUBLICATIONS
Author/co-author of more than 50 peer-reviewed scientific articles and technical reports.

- Varma, S; Rogers, DM; Pratt, LR; and **SB Rempe**. 2011. Design principles for K^+ selectivity in membrane transport. *J. Gen. Physiol. (Perspectives on Ion Selectivity)* 137:479-88 (invited).
- Alam, TM; Hart, D; and **SLB Rempe**. 2011. Computing the ^{7}Li NMR chemical shielding of hydrated Li^+ using cluster calculations and time-averaged configurations from ab initio molecular dynamics simulations. *Phys. Chem. Chem. Phys.* 13:13629 (**back cover**).
- Jiao, D; and **SB Rempe**. 2011. CO_2 solvation free energy using quasi-chemical theory. *J. Chem. Phys.* 134:224506-17.
- Rogers, DM; and **SB Rempe**. 2011. Probing the thermodynamics of competitive ion binding using minimum energy structures. *J. Phys. Chem. B* 115:9116–9129.
- Davis, RW; Kozina, CL; Jones, HDT; Branda, S; Sinclair, M; Singh, S and **SB Rempe**. 2011. Environmental perturbations to fluorescent proteins allow unambiguous discrimination of constructs with identical sequence. *Physical Biology* (invited; submitted).
- Rogers, DM; Beck, TL; and **SB Rempe**. 2011. Information theory and statistical mechanics revisited. *J. Statistical Phys.* (arXiv:1105.5662v1) (invited; submitted).
- Rogers, DM; and **SB Rempe**. 2011. A first and second law for nonequilibrium thermodynamics: Maximum entropy derivation of the fluctuation-dissipation theorem and entropy production functionals. *Phys. Rev. E* (arXiv:1105.5619v1) (submitted).
- Rogers, DM; and **SB Rempe**. 2011. Thermodynamic analyses of membrane separations processes. *Sandia Technical Report* (SAND2011:1759J).
- Yang, S; Jiang, Y-B; Chen, Z; Rogers, DM; Wang, Y; Brinker, CJ; and **SB Rempe**. 2011. Biomimetic high-flux desalination membrane based on self-assembled nanopores tuned by atomic layer deposition. *Sandia Technical Report* (SAND2010:6735).
- Jiao, D; Leung, K; **Rempe, SB**; and TM Nenoff. 2011. First principles calculations of atomic nickel redox potentials and dimerization free energies: A study of metal nanoparticle growth. *J. Chem. Theory Comput,* 7:485-495.
- Varma, S; and **SB Rempe**. 2010. Multi-body effects in ion binding and selectivity. *Biophys J* 99:3394.
- Asthagiri, D; Dixit, PD; Merchant, S; Paulaitis, M; Pratt, LR; **Rempe, SB**; and S Varma. 2010. Ion selectivity from local configurations of ligands in solutions and ion channels. *Chemical Physics Letters (Frontiers Article)* 485:1-7 (invited, **cover**, dedicated feature on journal website).
- **Rempe, SB**; and K Leung. 2010. Response to "Comment on 'Ab initio molecular dynamics calculation of ion hydration free energies' [JCP 133, 047103 (2010)]." *J. Chem. Phys.* 133:047104.
- Davis, RW; Aaron, JS; **Rempe, SL**; and JA Timlin. 2010. Fluorescence fluctuation analysis of mixed chromophores from a line-scanning hyperspectral imaging system. *Proc. SPIE* 7570 (757002):1-11.
- Lorenz, CD; Tsige, M; **Rempe, SB**; Chandross, M; Stevens, MJ; Grest, GS. 2010. Simulation study of the silicon oxide and water interface. *J. Comput. and Theoretical Nanoscience* 7(12):2586-2601 (invited).
- Clawson, JS; Leung, K; Cygan, RT; Alam, TM; and **SB Rempe**. 2010. Ab initio study of hydrogen storage in water clathrates. *J. Comput. and Theoretical Nanoscience* 7(12):2602-2606 (invited).
- Leung, K; and **SB Rempe**. 2009. Ion rejection by nanoporous membranes in pressure-driven molecular dynamics simulations. *J. Comput. and Theoretical Nanoscience* 6:1948-1955 (invited).
- Leung, K; **Rempe, SB**; and A von Lilienfeld. 2009. Ab initio molecular dynamics calculation of ion hydration free energies. *J. Chem. Phys*. 130 (20):204507-18.
- **Rempe, SB**; Mattsson, TR; Leung, K. 2008. On 'the complete basis set limit' and plane-wave methods in first-principles simulations of water. *Phys. Chem. Chem. Phys. (Communication)* 10:4685-87.
- Varma, S; and **SB Rempe**. 2008. Structural transitions in coordination preferences of ions. *J. Am. Chem. Soc.* 130 (56):15405-15419.
- Cygan, RT; Brinker, CJ; Nyman, M; Leung, K.; and **SB Rempe**. 2008. A molecular basis for advanced materials in water treatment. *Mater. Res. Soc. Bulletin* 33:42-47.
- Varma, S; Sabo, D; and **SB Rempe**. 2008. K^+/Na^+ selectivity in K-channels and valinomycin: Over-coordination versus cavity-size constraints. *J. Molec. Biol.* 376:13-22.

- Sabo, D; Varma, S; Martin, MG; and **SB Rempe**. 2008. Studies of the thermodynamic properties of hydrogen in bulk water. *J. Phys. Chem. B* 112:867-876.
- Whitfield, T; Varma, S; Harder, E; Lamoureux, G, **Rempe, SB** and B Roux. 2007. Theoretical study of aqueous solvation of K^+ comparing ab initio, polarizable, and fixed-charge models. *J. Chem. Theory Comput.* 3(6):2068-2082.
- Varma, S; and **SB Rempe**. 2007. Tuning ion coordination architectures to enable selective partitioning. *Biophysical J.* 93:1093-1099.
- Varma, S; and **SB Rempe**. 2006. Coordination numbers of alkali metal ions in aqueous solution. *Biophys. Chemistr*y 124:192-199 (invited).
- Leung, K; and **SB Rempe**. 2006. Ab initio rigid water: Effect on water structure, ion hydration, and thermodynamics. *Phys. Chem. Chem. Phys.* 8:2153-2162.
- Leung, K; **Rempe, SB**, *et al.* 2006. Density functional theory and DFT+U study of transition metal porphines adsorbed on Au (111) surfaces and effects of applied electric fields. *J. Am. Chem. Soc.* 128:3659-3668.
- Sabo, D; **Rempe, SB**; Greathouse, JA; and MG Martin. 2006. Molecular structure of hydrogen gas in bulk water. *Molecular Simulation* 32:269-278.
- Leung, K; **Rempe, SB**; and CD Lorenz. 2006. Salt permeation and exclusion in hydroxylated and functionalized silica pores. *Phys. Rev. Lett.* 96:095504.
- Leung, K; and **SB Rempe**. 2005. Ab initio molecular dynamics study of glycine intramolecular proton transfer in water. *J. Chem. Phys.* 122:184506-18.
- Leung, K; and **SB Rempe**. 2004. Ab initio molecular dynamics study of formate ion hydration. *J. Am. Chem. Soc.*126:1285-1289.
- **Rempe, SB**; Asthagiri, D and LR Pratt. 2004. Inner shell definition and absolute hydration free energy of K^+(aq) on the basis of quasi-chemical theory and ab initio molecular dynamics. *Phys. Chem. Chem. Phys.* 6:1966-1969.
- Asthagiri, D; Pratt, LR; Paulaitis, ME; and **SB Rempe.** 2004. Hydration structure and free energy of biomolecularly specific aqueous dications, including Zn^{2+} and first transition row metals. *J. Am. Chem. Soc.* 126:344-351.
- Ashbaugh, HS; Asthagiri, D; Pratt, LR and **SB Rempe**. 2003. Hydration of krypton and consideration of clathrate models of hydrophobic effects from the perspective of quasi-chemical theory. *Biophys. Chem*. 105:323-338.
- Tsige, M; Soddemann, T; **Rempe, SB**; *et al.* 2003. Interactions and structure of poly(dimethylsiloxane) at silicon dioxide surfaces. *J. Chem. Phys.* 118:5132-42.
- **Rempe, SB** and LR Pratt. 2001. The hydration number of Na^+ in liquid water. *Fluid Phase Equilibria* 183:121-132.
- **Rempe, SB**; Pratt, LR; Hummer, G; Kress, JD; Martin, RL and A Redondo. 2000. The hydration number of Li^+ in liquid water. *J. Am. Chem. Soc*. *(Letter)* 122:966-967.
- **Rempe, SB** and RO Watts. 1998. The exact quantum mechanical kinetic energy operator in internal coordinates for vibration of a hexatomic molecule. *J. Chem. Phys*. 108:10084-95.
- **Rempe, SB**; and H Jonsson. 1998. A computational exercise illustrating molecular vibrations and normal modes. *The Chemical Educator* 3:04231-6.
- **Rempe, SB** and RO Watts. 1997. The convergence properties of hindered rotor energy levels. *Chem. Phys. Lett.* 269:455-463.
- Gyorgyi, L; **Rempe, SL**; and RJ Field. 1991. A novel model for the simulation of chaos in low-flow-rate CSTR experiments with the Belousov-Zhabotinsky reaction. *J. Phys. Chem.* 95:3159-3165.

Selected Technical Reports, Book Chapters, Editorials, and Public Communications

- **Rempe, SB**; *et al.* 2010. Computational and experimental platform for understanding and optimizing water flux and salt rejection in nanoporous membranes. *Sandia Technical Report* (SAND2010-6735).
- **Rempe, SB**; Varma, S; Sabo, D; and S Singh. 2008. Block-mediated control of flux in ion channels. *Sandia Technical Report* (SAND2007-6315).
- **Rempe, SB**. 2007. How nature discriminates between Na^+ and K^+. *Science Matters.* (Sandia).
- **Rempe, SB**; and B Roux. 2006. Editorial for special issue on ions. *Biophys. Chemistr*y 124:169-170.

- Pratt, LR; Asthagiri, D; and **SB Rempe**. 2006. Momentum truncation errors and inferences of Li^+ hydration number on the basis of neutron diffraction from aqueous solutions. *Sandia Technical Report* (SAND2005-5371J).
- **Rempe, SB** and LR Pratt. 2000. Ion hydration and exchange studies aimed at ion channel selectivity. *Theoretical Division External Review* (Los Alamos National Laboratory).
- Jarvinen, GB; *et al.* 2000. Robust membrane systems for actinide separations, in *Plutonium Futures – The Science* (AIP Conf Proc 532:71-72).
- Pratt, LR and **SB Rempe**. 1999. Quasi-chemical theory and implicit solvent models for simulations, in *Simulation and Theory of Electrostatic Interactions in Solution* (AIP Conf Proc 492:172-201).